Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: R Gitomer Examiner # :_____ Date: 6/16/04
Art Unit: 1651 Phone Number 30_____ Serial Number: 09/995,757
Mail Box and Bldg/Room Location: _____ Results Format Preferred (circle): PAPER DISK E-MAIL
3671

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

****

STAFF USE ONLY	**Type of Search**	**Vendors and cost where applicable**
Searcher: Noble	NA Sequence (#)_____	STN 4138
Searcher Phone #: _____	AA Sequence (#)_____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: 6/24/04	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: 30	Fulltext _____	Sequence Systems _____
Clerical Prep Time: 0	Patent Family _____	WWW/Internet _____
Online Time: 270	Other _____	Other (specify)_____

STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 12[illegible]

TO: Ralph J Gitomer **Location: rem/3d65/3e71** **Art Unit: 1651** **Thursday, June 24, 2004** **Case Serial Number: 09/995737**	**From: Noble Jarrell** **Location: Biotech-Chem Library** **Rem 1B71** **Phone: 272-2556** **Noble.jarrell@uspto.gov**

Search Notes

STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact ***the searcher or contact:***

Mary Hale, Information Branch Supervisor
Remsen Bldg. 01 D86
571-272-2507

Voluntary Results Feedback For

- *I am an examiner in Workgroup:* ☐ *Example: 1610*
- *Relevant prior art* ***found****, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

  Types of relevant prior art found:
  - ☐ Foreign Patent(s)
  - ☐ Non-Patent Literature
    (journal articles, conference proceedings, new product announcements etc.)
- *Relevant prior art* ***not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC-Biotech-Chem Library Remsen Bldg.

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     FILE 'HCAPLUS' ENTERED AT 08:12:40 ON 24 JUN 2004
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L3   (        14)SEA FILE=HCAPLUS ABB=ON  PLU=ON  VIBRATIONAL OPTICAL ACTIVITY/C
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L5   (       606)SEA FILE=HCAPLUS ABB=ON  PLU=ON  MUTAROTATION/CT
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L18              3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND (PY<=2001 OR PRY<=2001
L19            354 CIRCULAR DICHROISM SPECTROSCOPY/CT
L20           1782 COTTON EFFECT+OLD/CT
L21          18368 CIRCULAR DICHROISM+OLD,NT/CT
L22           3995 OPTICAL ROTATORY DISPERSION+OLD/CT
L23          57378 SPECTROMETERS+OLD,NT/CT
L24           1711 POLARIZED LIGHT/CT
L25            380 POLARIZED LUMINESCENCE/CT
L26          62854 POLARIZATION+OLD,NT/CT
L27           1330 L23-26 (L) (CIRCUL? OR ROTAT?)
L28              0 L7-9 AND L10 AND (L19 OR L20 OR L21 OR L22 OR L27)
L29             80 L7-9 AND L10
L30           4393 L23-26 (L) OPTIC?
L31              0 L29 AND L30
L32              8 L29 AND (?CIRCUL? OR ?OPTIC? (1A) ?ROTAT? OR ?POLAR? OR ?OPTIC?
L33              5 L32 NOT (L11 OR L18)
L34          25839 REAGENTS+NT/CT
                   E BUCKE C/AU
L35            121 E3-7
                   E ADLARD M/AU
L36             49 E4-8
                   E SINGLETON V/AU
L37              7 E3,E13
                   E HORN J/AU
L38             76 E3,E13,E56-57
L39             52 OPTICAL ACT?/CS,PA
L40           3056 L34 (L) ANST+NT/RL
L41             57 L40 AND L10
L42              1 L41 AND L35-38
L43              0 L41 AND L39
L44             56 L41 NOT L42
L45             49 L44 AND (PY<=2001 OR AY<=2001 OR PRY<=2001 OR AD<20011129 OR PD
L46              9 L45 AND L7-9
L47             26 (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L16 OR L19 OR L20 OR L21 O
L48              1 L47 AND L35-38
L49              0 L47 AND L39
L50             25 L47 NOT L48
L51             17 L50 AND (PY<=2001 OR AY<=2001 OR PRY<=2001 OR AD<20011129 OR PD
L52              0 L18 AND L34
L53              1 L51 AND DICHROISM DETECTION/TI
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L54          72 (L1 OR L2 OR L3 OR L5 OR L6 OR L16 OR L19 OR L19 OR L20 OR L21
L55          71 L54 NOT L35-38
L56           0 L55 AND L39
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L58           2 L57 AND (STRUCTURE ELUCIDATION OR OPTICAL ROTATION)/TI
L59          63 L57 NOT L58
L60           2 L59 AND (SOLUBILITY-PH OR CIRCULAR DICHROISM)/TI
L61          61 L59 NOT L60
L62           4 L58 OR L60
L63         218 (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L16 OR L19 OR L20 OR L21 O
L64           1 L63 AND L35-38
L65           0 L63 AND L39
L66         217 L63 NOT L64
L67         147 L66 AND (PY<=2001 OR AY<=2001 OR PRY<=2001 OR PD<20011129 OR AD
L68           6 L67 AND (INCLUSION COMPLEXATION OR AFFINITY SEPARATION OR PURIF
L69         141 L67 NOT L68
L70          10 L69 AND (SPECTROSCOPIC PROBES OR BIREFRINGENCE OR CONCENTRATION
L71           6 L70 NOT (CHIRAL OR GENERIC ALGORITHMS)/TI
L72           4 L70 NOT L71
L73           1 L72 AND BIREFRINGENCE/TI
L74           7 L71 OR L73
L75           5 L35-38 AND DEXTRAN/TI
                SEL AN DN 3-5
L76           3 E1-9 AND L75
                SEL RE L76
L77          18 E10-28
L78           2 L77 AND (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L16 OR L19 OR L20
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L80           6 L74 NOT GENETIC ALGORITHMS/TI
L81      114658 (?OPTIC? (L) (ROTAT? OR ACTIVIT?) OR CIRCUL? (L) DICHRO? OR ?PO
L82        2330 L81 AND ?STANDARD?/BI
L83         394 L82 AND ?CONCENTRAT?/BI
L84          33 L83 AND (L34 OR ?REAG?/BI)
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L86           0 L84 AND L39
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L89           9 L88 AND (POLARIMETRIC OR AROMATIZING OR SUCROSE OR OCTACOORDINA
                SEL AN  2-5
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                SEL AN 3
L91           1 E9-10 AND L90

=> b hcap
FILE 'HCAPLUS' ENTERED AT 12:00:47 ON 24 JUN 2004
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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:413992 HCAPLUS
DN 138:378287
ED Entered STN: 30 May 2003
TI A method for the measurement of the concentration of a material such as dextran or raffinose in a solution
IN Bucke, Christopher; Adlard, Max; Singleton, Victoria; Horn, Jennifer
PA UK
SO U.S. Pat. Appl. Publ., 9 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C12Q001-34
ICS C12N009-24
NCL 435018000; 435200000
CC 80-6 (Organic Analytical Chemistry)
Section cross-reference(s): 9, 11, 17
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003100041	A1	20030529	US 2001-995737	20011129
	GB 2367617	A1	20020410	GB 2000-24299	20001004
	GB 2367617	B2	20040107		
PRAI	US 2001-995737	A	20011129		

AB A method for the measurement of the concentration of a material such as dextran or raffinose in a solution, notably a sugar solution, comprises the step of: i measurement of the optical rotation of a solution sample; ii treatment of the sample with a reactive agent, reactive with the material, sufficient to alter the optical rotation of the sample; iii measurement of the optical rotation of the sample after treatment; and iv calcn. of the concentration of the material by reference to a suitable standard

ST assay
IT Wavelength
(IR; method for measurement of concentration of a material such as dextran or raffinose in a solution)
IT Fruit and vegetable juices
(cane; method for measurement of concentration of a material such as dextran or raffinose in a solution)
IT Samples
(liquid; method for measurement of concentration of a material such as dextran or raffinose in a solution)
IT **Concentration (condition)**
Materials
Mathematical methods
Molecular weight
Optical activity
Particle size
Polarimetry
Solids

Solutions
Standard substances, analytical
Test kits
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

IT Carbohydrates, analysis
RL: ANT (Analyte); ANST (Analytical study)
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

IT Reagents
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

IT Diatomite
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

IT 57-50-1, Sucrose, analysis 512-69-6, Raffinose 9000-69-5, Pectin
9004-53-9, Dextrin 9004-54-0, Dextran, analysis 9014-63-5, Xylan
RL: ANT (Analyte); ANST (Analytical study)
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

IT 9025-35-8, α-Galactosidase 9025-70-1, Dextranase
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(method for measurement of concentration of a material such as dextran or raffinose in a solution)

=> d all l53 tot

L53 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:814738 HCAPLUS
DN 134:2319
ED Entered STN: 21 Nov 2000
TI Reagent and process for peptide/protein differentiation using circular **dichroism detection**
IN Purdie, Neil; Province, Dennis William
PA The Board of Regents for Oklahoma State University, USA
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N033-68
CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6, 80
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000068695	A2	20001116	WO 2000-US13246	20000512 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 1999-134017P P 19990512 <--
AB A reagent comprised of an aqueous solution of Cu(II)-D-histidine complex acts effectively as a devitalizing agent required to qual. identify an

enantiomer and quant. determine its enantiomeric purities. The initial function of the host ligand (D-histidine) is to keep the Cu(II) ion in solution in high pH values. The base line CD spectrum associated with each Cu-(chiral ligand) host complex is uniquely different. On adding peptide or protein, exchange occurs between the host ligand (D-histidine) in the analyte ligand (protein). Exchanges produce changes in the CD spectrum that are significant enough that they have the potential of becoming a reliable spectroscopic fingerprint for every individual analyte.

ST reagent peptide protein differentiation CD; copper histidine complex CD peptide protein

IT Proteins, specific or class
RL: ANT (Analyte); FMU (Formation, unclassified); PRP (Properties); ANST (Analytical study); FORM (Formation, nonpreparative)
(complexes, with copper; reagent and process for peptide/protein differentiation using CD detection)

IT Peptides, analysis
RL: ANT (Analyte); FMU (Formation, unclassified); PRP (Properties); ANST (Analytical study); FORM (Formation, nonpreparative)
(copper complexes; reagent and process for peptide/protein differentiation using CD detection)

IT Algorithm
Circular dichroism
Pharmaceutical analysis
Principal component analysis
(reagent and process for peptide/protein differentiation using CD detection)

IT Peptides, analysis
Proteins, general, analysis
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); ANST (Analytical study); PROC (Process); RACT (Reactant or reagent)
(reagent and process for peptide/protein differentiation using CD detection)

IT **Reagents**
RL: **ARG (Analytical reagent use)**; RCT (Reactant); **ANST (Analytical study)**; RACT (Reactant or reagent); USES (Uses)
(reagent and process for peptide/protein differentiation using CD detection)

IT Protein sequences
(validation of; reagent and process for peptide/protein differentiation using CD detection)

IT 7681-11-0, Potassium iodide, analysis
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(as stabilizer in reagent solution; reagent and process for peptide/protein differentiation using CD detection)

IT 9004-10-8, Insulin, analysis
RL: ANT (Analyte); PRP (Properties); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)
(of human and bovine and porcine and recombinant; reagent and process for peptide/protein differentiation using CD detection)

IT 556-50-3D, complex with Cu(II) 658-79-7D, complex with Cu(II)
673-08-5D, complex with Cu(II) 687-69-4D, complex with Cu(II)
691-81-6D, complex with Cu(II) 730-08-5D, complex with Cu(II)
1050-28-8D, complex with Cu(II) 1187-50-4D, complex with Cu(II)
1948-31-8D, complex with Cu(II) 3061-88-9D, complex with Cu(II)
3695-73-6D, complex with Cu(II) 6234-26-0D, complex with Cu(II)
7451-76-5D, complex with Cu(II) 7758-33-0D, complex with Cu(II)
14857-82-0D, complex with Cu(II) 18625-22-4D, complex with Cu(II)
19729-30-7D, complex with Cu(II) 21778-69-8D, complex with Cu(II)
69242-40-6D, complex with Cu(II) 86030-53-7D, complex with Cu(II)

306275-69-4D, complex with Cu(II)
RL: ANT (Analyte); FMU (Formation, unclassified); PRP (Properties); ANST (Analytical study); FORM (Formation, nonpreparative)
(reagent and process for peptide/protein differentiation using CD detection)

IT 556-50-3 658-79-7 673-08-5 687-69-4 691-81-6 730-08-5 1050-28-8 1187-50-4, L-Leucylglycylglycine 1948-31-8 3061-88-9 3695-73-6 6234-26-0, Glycylglycyl-L-phenylalanine 7451-76-5, Glycylglycyl-L-histidine 7758-33-0, Glycyl-L-histidylglycine 8049-62-5, Zinc insulin 14857-82-0, Glycylglycyl-L-leucine 18625-22-4, D-Leucylglycylglycine 19729-30-7, Glycylglycyl-L-alanine 21778-69-8, L-Tyrosylglycylglycine 69242-40-6, Glycylglycyl-L-isoleucine 86030-53-7 306275-69-4
RL: ANT (Analyte); PRP (Properties); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)
(reagent and process for peptide/protein differentiation using CD detection)

IT 6341-24-8, D-Histidine hydrochloride
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(reagent and process for peptide/protein differentiation using CD detection)

IT 15158-11-9DP, Copper 2+, complex with peptides, preparation 308321-67-7P
RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(reagent and process for peptide/protein differentiation using CD detection)

IT 60617-12-1D, β-Endorphin, complexes with copper(II)
RL: PRP (Properties)
(reagent and process for peptide/protein differentiation using CD detection)

IT 351-50-8, D-Histidine 1310-73-2, Sodium hydroxide, uses 7758-98-7, Copper sulfate, uses
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(reagent solution containing; reagent and process for peptide/protein differentiation using CD detection)

=> d all l62 tot

L62 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:566862 HCAPLUS
DN 135:132414
ED Entered STN: 06 Aug 2001
TI Method and device for measurement of **solubility-pH** profiles for drug screening
IN Avdeef, Alex; Tsinman, Konstantin L.
PA Pion, Inc., USA
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N021-33
CC 1-1 (Pharmacology)
Section cross-reference(s): 9
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001055698	A1	20010802	WO 2001-US2377	20010125 <--
W: JP				

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR
US 2002004244 A1 20020110 US 2001-769570 20010125 <--
US 6569686 B2 20030527
EP 1250587 A1 20021023 EP 2001-903291 20010125 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR
JP 2003521686 T2 20030715 JP 2001-555790 20010125 <--
PRAI US 2000-178616P P 20000128 <--
WO 2001-US2377 W 20010125 <--

AB The measurement of aqueous solubility in a high-throughput screening environment plays an important role in the selection of the most promising drug candidate mols. in pharmaceutical research and development. The invention describes a method, a simple, robust, high-throughput screen, that is applicable for the determination of the equilibrium solubility of sparingly soluble compds. and that may be used in pharmaceutical, biotechnol., and related industries. An anal. device has been designed to implement the solubility measurement technique. The basic method involves determining solubility of a compound by measuring the UV spectrum of a reference solution of the compound, under conditions avoiding or suppressing precipitation, and comparing it to the UV spectrum of a saturated sample solution of the compound Variations of the basic method include: (a) making reference solns. either by dilution of the sample solution to the point where precipitation is avoided, or by adding a water-miscible cosolvent to the sample solution so that precipitation is suppressed, and comparing the UV absorbances of the compound under reference conditions to the compound in a saturated solution, (b) determining the true aqueous solubility from the effect on the pKa that results from dissolving the compound in an aqueous solution containing some DMSO (typically 0.1-5% volume/volume), and (c) correcting concns. determined from the UV absorbance values for impurities.

ST app drug screening soly pH profile
IT Self-association
Surfactants
(anomaly caused by; solubility-pH profile method and apparatus for drug screening)
IT Bile acids
Phospholipids, miscellaneous
RL: MSC (Miscellaneous)
(anomaly caused by; solubility-pH profile method and apparatus for drug screening)
IT **Spectrometers**
(**circular** dichrometers; solubility-pH profile method and apparatus for drug screening)
IT Solvents
(cosolvents; solubility-pH profile method and apparatus for drug screening)
IT Ion pairs
(ion pair-forming counterions, anomaly caused by; solubility-pH profile method and apparatus for drug screening)
IT Counterions
(ion pair-forming, anomaly caused by; solubility-pH profile method and apparatus for drug screening)

α-crystallin is best classified as a mixed protein. In addition, increased temperature and concentration of α-crystallin result in increased α-helixes with a compensatory decrease in β-sheets. Such structural alterations in α-crystallin may be functionally important during terminal differentiation of the lens fiber cells that is accompanied by increased protein concns. and its role as a chaperone-like protein.

ST crystallin alpha secondary structure UV CD

IT **Concentration (condition)**
Secondary structure
α-Helix
β-Sheet
(effects of temperature and concentration on bovine lens α-crystallin secondary structure: CD spectroscopic study)

IT **Circular dichroism**
(far UV; effects of temperature and concentration on bovine lens α-crystallin secondary structure: CD spectroscopic study)

IT Temperature effects, biological
(heat; effects of temperature and concentration on bovine lens α-crystallin secondary structure: CD spectroscopic study)

IT Crystallins
RL: PRP (Properties)
(α-; effects of temperature and concentration on bovine lens α-crystallin secondary structure: CD spectroscopic study)

=> d all l91 tot

L91 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1964:31815** HCAPLUS
DN 60:31815
OREF 60:5724h,5725a-c
ED Entered STN: 22 Apr 2001
TI Determination of **sucrose**, invert sugar, and raffinose in sugar solutions
AU Oikawa, S.
SO Seito Gijutsu Kenkyu Kaishi (**1962**), 11, 28-37
From: Sugar Ind. Abstr. 25(4), Abstr. No. 273(1963).
CODEN: SGIKA6; ISSN: 0370-9841
DT Journal
LA Unavailable
CC 50 (Industrial Carbohydrates)
AB Beet products from Japanese factories may contain appreciable amts. of invert sugar. The method of double polarization (according to Jackson and Gillis, method III) and the paper chromatographic method of de Whalley as modified by Albon and Gross were compared for the analysis of beet molasses or thick juice. The paper chromatographic method was used in conjunction with the determination of total sugars by Ofner's method after inversion. Invert sugar was determined by Ofner's method in both cases. The normal solution was clarified before polarization by adding a neutral Pb acetate solution (40 ml. in 200 ml.) and de-leading with NH4 phosphate, followed if necessary by decolorization of 20 ml. of normal solution in a column of Amberlite IRA-401 resin (Cl form) at 80° and dilution to 100 or 110 ml. Zn dust was used in some cases to decolorize the solution after acid inversion. The chromatograms were sprayed with naphtho-resorcinol **reagent** and dried at 90° for 10 min. The mean diameter of the raffinose spot (4-5 mm. on the starting line, for a 2-μl. volume) increased linearly with increasing **concentration** of raffinose over the range 0.4-0.8°. Three **standard** spots of different known

concns. were prepared for comparison. The error of the paper chromatographic determination of raffinose was ≤ 10%. The double polarization method gave results in good agreement with theory, except in cases where the sp. **optical rotation** of invert sugar was abnormal owing to an increase in the ratio of glucose to fructose; in such cases the paper chromatographic method should be applied in order to calculate the polarization equivalent of the reducing sugars.

IT Sugars
(analysis, determination of invert sugar, raffinose and **sucrose** in sugar-manufacturing solns.)

IT 512-69-6, Raffinose 8013-17-0, Sugar, invert
(determination of, in sugar-manufacturing solns.)

=> b home
FILE 'HOME' ENTERED AT 12:01:50 ON 24 JUN 2004

IT Ionization
(ionizable compds.; solubility-pH profile method and apparatus for drug screening)
IT Spectrometers
(light-scattering; solubility-pH profile method and apparatus for drug screening)
IT Polymers, miscellaneous
RL: MSC (Miscellaneous)
(non-ionizable, anomaly caused by; solubility-pH profile method and apparatus for drug screening)
IT **Optical activity**
Sensors
(optical rotation; solubility-pH profile method and apparatus for drug screening)
IT Acidity
(pKa; solubility-pH profile method and apparatus for drug screening)
IT Apparatus
Buffers
Circular dichroism spectroscopy
Colorimeters
Colorimetry
Drug screening
Filtration
Fluorometers
Fluorometry
Light scattering
Polarimeters
Polarimetry
Precipitation (chemical)
Solubility
Spectrometers
Spectrophotometry
Standard solutions, analytical
Titration
UV and visible spectrometers
UV and visible spectroscopy
pH
(solubility-pH profile method and apparatus for drug screening)
IT Polyoxyalkylenes, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solubility-pH profile method and apparatus for drug screening)
IT 12619-70-4, Cyclodextrin
RL: MSC (Miscellaneous)
(anomaly caused by; solubility-pH profile method and apparatus for drug screening)
IT 50-48-6, Amitriptyline 50-53-3, Chlorpromazine, biological studies 53-86-1, Indomethacin 54-31-9, Furosemide 57-66-9, Probenecid 72-69-5, Nortriptyline 93-09-4, 2-Naphthoic acid 94-78-0, Phenazopyridine 126-07-8, Griseofulvin 525-66-6, Propranolol 2609-46-3, Amiloride 15307-86-5, Diclofenac 22916-47-8, Miconazole 36322-90-4, Piroxicam 50679-08-8, Terfenadine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(solubility-pH profile method and apparatus for drug screening)
IT 67-68-5, DMSO, uses
RL: MSC (Miscellaneous); NUU (Other use, unclassified); USES (Uses)
(solubility-pH profile method and apparatus for drug screening)

IT 57-55-6, Propylene glycol, uses 64-17-5, Ethanol, uses 64-19-7, Acetic acid, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 68-12-2, Dimethylformamide, uses 71-23-8, 1-Propanol, uses 75-05-8, Acetonitrile, uses 79-14-1, Glycolic acid, uses 107-21-1, Ethylene glycol, uses 107-35-7, Taurine 109-99-9, Tetrahydrofuran, uses 123-91-1, 1,4-Dioxane, uses 127-09-3, Sodium acetate 4432-31-9, MES 7365-45-9, HEPES 7732-18-5, Water, uses 10043-35-3, Boric acid, uses 25322-68-3, Polyethylene glycol 145224-94-8
RL: NUU (Other use, unclassified); USES (Uses)
(solubility-pH profile method and apparatus for drug screening)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Bevan, C; WO 9913328 A 1999 HCAPLUS
(2) Lipinski, C; ADVANCED DRUG DELIVERY REVIEWS 1997, V23(1/03), P3
(3) Meserole, F; US 4906580 A 1990

L62 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:497393 HCAPLUS
DN 131:282611
ED Entered STN: 11 Aug 1999
TI **Structure Elucidation** of the Adducts Formed by Fjord-Region Dibenzo[a,l]pyrene 11,12-Dihydrodiol 13,14-Epoxides and Deoxyadenosine
AU Li, Kai-Ming; George, Mathai; Gross, Michael L.; Seidel, Albrecht; Luch, Andreas; Rogan, Eleanor G.; Cavalieri, Ercole L.
CS Eppley Institute for Research in Cancer and Allied Diseases, University of Nebraska Medical Center, Omaha, NE, 68198-6805, USA
SO Chemical Research in Toxicology (**1999**), 12(9), 758-767
CODEN: CRTOEC; ISSN: 0893-228X
PB American Chemical Society
DT Journal
LA English
CC 4-6 (Toxicology)
Section cross-reference(s): 9
AB Model adducts to be used in the identification of biol. formed adducts were synthesized by reaction of fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides (DB[a,l]PDE) and deoxyadenosine (dA). The (±)-anti-DB[a,l]PDE was reacted with dA in DMF at 100 °C for 30 min to give four DB[a,l]PDE-14-N6dA adducts: (-)-anti-trans (26%), (+)-anti-trans (26%), (-)-anti-cis (17%), and (+)-anti-cis (17%). The (±)-syn-DB[a,l]PDE was reacted with dA under the same conditions to yield four DB[a,l]PDE-14-N6dA adducts and one N7Ade adduct: (+)-syn-cis (19%), (+)-syn-trans (13%), (-)-syn-cis (19%), (-)-syn-trans (13%), and (±)-syn-DB[a,l]PDE-14-N7Ade (22%). The structures of the eight stereoisomers of DB[a,l]PDE-14-N6dA were unequivocally assigned by reacting optically pure (-)-anti-DB[a,l]PDE and (+)-syn-DB[a,l]PDE with dA and by a combination of NMR, CD, and fast atom bombardment mass spectrometry. Reactions at 100 °C yielded mainly the trans-opened adducts at the benzylic C-14 position for both (±)-anti-DB[a,l]PDE and (-)-anti-DB[a,l]PDE, whereas (±)-syn-DB[a,l]PDE and (+)-syn-DB[a,l]PDE afforded mainly cis-opened adducts. At room temperature, however, only trans-opened adducts were obtained from (±)-anti-DB[a,l]PDE and only cis-opened adducts from (±)-syn-DB[a,l]PDE. Steric hindrance created by the fjord region may be an important factor for the stereoselectivity observed at room temperature
ST DNA adduct dibenzopyrenedihydrodiol epoxide deoxyadenosine structure; mol model DNA adduct dibenzopyrenedihydrodiol epoxide deoxyadenosine structure; Fjord region DNA adduct dibenzopyrenedihydrodiol epoxide deoxyadenosine structure

IT DNA
RL: ADV (Adverse effect, including toxicity); ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(adducts; structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT Xenobiotics
(metabolism, metabolic activation; structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT Carcinogens
Circular dichroism spectroscopy
Fast atom bombardment mass spectrometry
Genotoxicity
HPLC
Molecular modeling
NMR (nuclear magnetic resonance)
Neoplasm
Skin, neoplasm
Standard substances, analytical
Stereochemistry
(structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT 958-09-8D, Deoxyadenosine, adducts with dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides 158414-00-7D, DNA adducts
RL: ADV (Adverse effect, including toxicity); ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT 160180-24-5P 160180-27-8P 160227-19-0P 160227-20-3P 160227-21-4P 160227-22-5P 160227-23-6P 160227-24-7P 160227-25-8P
RL: ADV (Adverse effect, including toxicity); ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT 153857-28-4 153926-04-6 158414-00-7
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
IT 958-09-8, Deoxyadenosine
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structure elucidation of the adducts formed by Fjord-region dibenzo[a,l]pyrene 11,12-dihydrodiol 13,14-epoxides and deoxyadenosine)
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Agarwal, S; J Am Chem Soc 1987, V109, P2497 HCAPLUS
(2) Amin, S; Carcinogenesis 1995, V16, P1971 HCAPLUS
(3) Amin, S; Carcinogenesis 1995, V16, P2813 HCAPLUS
(4) Cavalicri, E; Carcinogenesis 1991, V12, P1939
(5) Cavalieri, E; J Cancer Res Clin Oncol 1989, V115, P67 MEDLINE
(6) Devanesan, P; Chem Res Toxicol 1999, V12, PXXX
(7) Devanesan, P; Chem Res Toxicol 1999, V12, PXXX

(8) Frank, H; Polycyclic Aromat Compd 1996, V10, P109 HCAPLUS
(9) Gill, H; Carcinogenesis 1995, V15, P2455
(10) Gross, M; Anal Chim Acta 1991, V250, P105 HCAPLUS
(11) Higginbotham, S; Carcinogenesis 1993, V14, P875 HCAPLUS
(12) LaVoie, E; Cancer Lett 1993, V70, P7 HCAPLUS
(13) Lambert, J; Organic Structural Analysis 1976
(14) Li, K; Biochemistry 1995, V34, P8043 HCAPLUS
(15) Li, K; Chem Res Toxicol 1999, V12, PXXX
(16) Luch, A; Chem Res Toxicol 1997, V10, P1161 HCAPLUS
(17) Ralston, S; Cancer Res 1994, V54, P887 HCAPLUS
(18) Ralston, S; Carcinogenesis 1995, V16, P2899 HCAPLUS
(19) RamaKrishna, N; Chem Res Toxicol 1993, V6, P554 HCAPLUS
(20) Szeliga, J; Chem Res Toxicol 1995, V8, P1014 HCAPLUS
(21) Thakker, D; Stereochemical Aspects of Pharmacologically Active Compounds 1988, P271
(22) US Government Printing Office; NIH Guidelines for the Laboratory Use of Chemical Carcinogens 1981

L62 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:554886 HCAPLUS
DN 83:154886
ED Entered STN: 12 May 1984
TI Recommended reference materials for realization of physicochemical properties. **Optical rotation**
CS IUPAC Physical Chemistry Division, UK
SO Pure and Applied Chemistry (**1974**), 40(3), 451-5
CODEN: PACHAS; ISSN: 0033-4545
DT Journal
LA English
CC 73-2 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
AB Sucrose, anhydrous dextrose, and quartz are recommended as reference materials for optical rotation detns.
ST optical rotation ref material
IT **Optical rotation**
(determination of, reference materials for)
IT **Standard substances**
(for optical rotation detns.)
IT 50-99-7, uses and miscellaneous 57-50-1, uses and miscellaneous 14808-60-7, uses and miscellaneous
RL: USES (Uses)
(reference material, for optical rotation detns.)

L62 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:487296 HCAPLUS
DN 71:87296
ED Entered STN: 12 May 1984
TI Suggested preliminary standards for calibration of optical rotatory dispersion and **circular dichroism** instruments
AU DeTar, DeLos F.
CS Florida State Univ., Tallahassee, FL, USA
SO Analytical Chemistry (**1969**), 41(11), 1406-8
CODEN: ANCHAM; ISSN: 0003-2700
DT Journal
LA English
CC 79 (Inorganic Analytical Chemistry)
AB Two approaches have been used in the present study in an effort to define preliminary circular dichroism (C.D.) standards. The 1st involved a careful reexamn. of 10-camphorsulfonic acid by using the Kronig-Kramers

transform to compare O.R.D. and C.D. curves. The 2nd approach utilized Co(en)3I3.H2O, a compound relatively easy to prepared and resolve and 1 for which 3 independent sets of absolute rotation values have been reported. Experience has shown that the angle measuring portion of a recording spectropolarimeter may not be in correct adjustment, and that the error may be a function of the full scale reading. This section of the instrument should, therefore, be checked against suitable O.R.D. standards before attempting to use O.R.D. value to establish a C.D. calibration. It is clearly undesirable to use ordinary uv or visible spectrometric values as a substitute for polarimetric values in deciding the optical purity of an intended standard.

ST standards circular dichroism; circular dichroism standards; ORD comparison circular dichroism; calibration circular dichroism; cobalt complexes circular dichroism; camphorsulfonic acid circular dichroism

IT Dichroism
(circular, preliminary standards for calibration in)

IT **Standard substances**
(for optical rotary dispersion)

IT **Optical rotatory dispersion**
(preliminary standards for calibration in)

IT Ethylenediamine, cobalt complexes
RL: PREP (Preparation)
(preparation of)

IT 5872-08-2 15405-85-3
RL: ANST (Analytical study)
(as preliminary standard for O.R.D.)

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L80 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:886617 HCAPLUS
DN 136:2464
ED Entered STN: 07 Dec 2001
TI System and method for the classification and of **biological samples** and their diagnostic potential
IN Norgaard, Lars; Albrechtsen, Morten; Olsen, Ole Ingemann; Harrit, Niels; Bro-Jorgensen, Rasmus
PA Medicometrics Aps, Den.
SO PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N021-64
ICS A61B005-00
CC 9-1 (Biochemical Methods)
Section cross-reference(s): 14
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001092859	A1	20011206	WO 2001-DK383	20010601 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1290428 A1 20030312 EP 2001-938006 20010601 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2003535330 T2 20031125 JP 2002-501018 20010601 <--
US 2003162301 A1 20030828 US 2003-297187 20030416 <--
PRAI DK 2000-863 A 20000602 <--
WO 2001-DK383 W 20010601 <--

AB The invention concerns a method of training a classification system for characterizing a biol. sample, a diagnostic classification system, as well as a method of characterizing a condition in an animal or a human being by using parameters obtained from the sample. The invention relates to classification based on phys. parameters obtained from luminescence spectroscopy on light emitted from the sample. The data obtained from a spectrofluorimetric anal. can be considered a finger-print of the sample. Each sample gives rise to a unique spectrofluorometric set of phys. parameters. By analyzing the fluorescence data, it is possible to classify samples into two or more classes based on the fluorescence spectra, such as classifying with respect to presence/absence of a specific disease, group of diseases or risk of later attaining a specific disease or a body condition, or concentration of a specific compound or medicine.

ST analytical app system classifying biomol disease diagnosis chromatog computer

IT Aging, animal
Analytical apparatus
Animal
Animal tissue
Anisotropy
Bile
Biochemical molecules
Blood analysis
Blood plasma
Blood serum
Body fluid
Brain
Cerebrospinal fluid
Computer application
Computer program
Concentration (condition)
Diagnosis
Disease, animal
Eubacteria
Fasting
Feces
Fluorescence
Fluorometry
Hair
Heart, disease
Human
Kidney
Light sources
Liver
Luminescence spectroscopy
Lymph
Milk analysis
Muscle
Narcotics
Phosphorescence
Polarization
Saliva

Semen
Sex
Simulation and Modeling, physicochemical
Skin
Statistical analysis
Stress, animal
Sweat
Tear (ocular fluid)
Temperature effects, biological
Tobacco smoke
Urine analysis
pH
(System and method for the classification and of biol. samples and their diagnostic potential)

IT Drugs of abuse
(abuse of; System and method for the classification and of biol. samples and their diagnostic potential)

IT Intestine, neoplasm
(colon; System and method for the classification and of biol. samples and their diagnostic potential)

IT **Circular dichroism**
(fluorescence-detected; System and method for the classification and of biol. samples and their diagnostic potential)

IT Mucus
(nasal; System and method for the classification and of biol. samples and their diagnostic potential)

IT Ecology
(population; System and method for the classification and of biol. samples and their diagnostic potential)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Instrumentation Metrics Inc; WO 0042907 A 2000
(2) O'Brien, K; IEEE TRANSACTIONS ON BIOMEDICAL ENGINEERING 1989, V36(4), P424 MEDLINE
(3) Rosenthal, R; US 5576544 A 1996 HCAPLUS
(4) University Of Texas; WO 9630746 A 1996
(5) University Of Texas; WO 9824369 A 1998

L80 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:310769 HCAPLUS
DN 133:89648
ED Entered STN: 14 May 2000
TI Measurements of **concentration dependence** and enantiomeric purity of terpene solutions as a test of a new commercial VCD spectrometer
AU Urbanova, Marie; Setnicka, Vladimir; Volka, Karel
CS Department of Physics and Measurement, Institute of Chemical Technology at Prague, Prague, 16628/6, Czech Rep.
SO Chirality (**2000**), 12(4), 199-203
CODEN: CHRLEP; ISSN: 0899-0042
PB Wiley-Liss, Inc.
DT Journal
LA English
CC 30-10 (Terpenes and Terpenoids)
Section cross-reference(s): 22
AB Vibrational CD (VCD) spectra of (+)-α-pinene solns. in carbon tetrachloride have been measured in the range of volume fractions 5-100% (volume/volume) in the mid-IR region. The concentration dependence measured was
statistically analyzed with the aim of obtaining a reliable correlation

between the VCD band areas and the concns. of individual enantiomers. The quality of the spectra was estimated by means of noise spectra which were defined as half the difference of the two following blocks of scans. In addition to this, the enantiomeric purity was studied. This study was carried out for both (+)- and (-)-α-pinene enantiomers in the range of the percent enantiomeric excess in the interval 10-100%. The relationship between VCD intensity and enantiomeric purity was determined by least-square regression and statistically evaluated. All measurements performed in this study were intended as a basic tool for testing of a new com. VCD setup from Bruker.

ST terpene soln concn dependence enantiomeric purity VCD spectra; pinene soln concn dependence enantiomeric purity VCD spectra; limonene soln concn dependence enantiomeric purity VCD spectra; borneol soln concn dependence enantiomeric purity VCD spectra; least square regression analysis concn dependence terpene soln; statistical analysis concn dependence enantiomeric purity terpene soln

IT **Concentration (condition)**
(dependence; measurements of concentration dependence and enantiomeric purity
of terpene solns. as a test of a new com. VCD spectrometer)

IT Purity
(enantiomeric; measurements of concentration dependence and enantiomeric purity of terpene solns. as a test of a new com. VCD spectrometer)

IT Regression analysis
(least-square; measurements of concentration dependence and enantiomeric purity of terpene solns. as a test of a new com. VCD spectrometer)

IT Statistical analysis
Vibrational circular dichroism
(measurements of concentration dependence and enantiomeric purity of terpene solns. as a test of a new com. VCD spectrometer)

IT Terpenes, properties
RL: PRP (Properties)
(measurements of concentration dependence and enantiomeric purity of terpene solns. as a test of a new com. VCD spectrometer)

IT 464-43-7, (+)-Borneol 464-45-9, (-)-Borneol 5989-27-5, (+)-Limonene 5989-54-8, (-)-Limonene 7785-26-4, (-)-α-Pinene 7785-70-8, (+)-α-Pinene
RL: PRP (Properties)
(measurements of concentration dependence and enantiomeric purity of terpene solns. as a test of a new com. VCD spectrometer)

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(8) Long, F; Appl Spectrosc 1997, V51, P504 HCAPLUS
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(10) Nafie, L; Enantiomer 1998, V3, P283 MEDLINE
(11) Nafie, L; Spectroscopy 1987, V2, P24 HCAPLUS
(12) Pancoska, P; Biochemistry 1989, V28, P5917 HCAPLUS
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(14) Polavarapu, P; Appl Spectrosc 1984, V38, P438 HCAPLUS
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(19) Wang, B; Appl Spectrosc 1995, V49, P1347 HCAPLUS

L80 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:667657 HCAPLUS
DN 131:331311
ED Entered STN: 20 Oct 1999
TI The magneto-chiral **birefringence** in diamagnetic solutions and in uniaxial crystals
AU Kalugin, Nikolai G.; Kleindienst, Peter; Wagniere, Georges H.
CS Institute of Physical Chemistry, University of Zurich, Zurich, CH-8057, Switz.
SO Chemical Physics (**1999**), 248(1), 105-115
CODEN: CMPHC2; ISSN: 0301-0104
PB Elsevier Science B.V.
DT Journal
LA English
CC 77-8 (Magnetic Phenomena)
Section cross-reference(s): 22, 73
AB The interferometric measurement of the magneto-chiral birefringence is reported in several chiral organic solns. and in the chiral uniaxial crystals α-quartz and LiIO3 at a wavelength of 633 nm and in static magnetic fields of up to 5 T. The tech. details of the exptl. procedure are described in P. Kleindienst and G. Wagniere [Chemical Phys. Lett. 288(1998) 89]. The results are in agreement with the predicted selection rules. The orders of magnitude correlate with those for natural optical rotation and magnetic optical rotation. An unexpected behavior is found in LiIO3 at fields .gtorsim.3 T, and its possible origins are discussed.
ST magnetochiral birefringence diamagnetic soln uniaxial crystal; interferometer chiral org soln quartz lithium iodate crystal; selection rule magnetic field optical rotation
IT Birefringence
Chirality
Concentration (condition)
Diamagnetism
Interferometry
Magnetic field effects
Optical activity
Selection rule
Solutions
(magneto-chiral birefringence in diamagnetic solns. and in uniaxial crystals)
IT 147-85-3, Proline, properties 663-17-2 13765-03-2, Lithium iodate (LiIO3) 14808-60-7, Quartz, properties 35193-63-6 208193-31-1
RL: PRP (Properties)
(magneto-chiral birefringence in diamagnetic solns. and in uniaxial crystals)
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

(1) Aldrich Chemie; Aldrich Catalogue 1996
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(3) Anon; Landolt-Bornstein, 6th ed 1950, V1(part 1), P409
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(16) Surma, M; Mol Phys 1997, V90, P993 HCAPLUS
(17) Surma, M; Mol Phys 1998, V93, P271 HCAPLUS
(18) The Chemical Rubber Co; Handbook of Chemistry and Physics, 45th ed 1964, PC484
(19) Wagniere, G; Chem Phys 1999, V245, P165 HCAPLUS
(20) Wagniere, G; Z Naturforsch 1984, V39a, P254 HCAPLUS

L80 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:636351 HCAPLUS
DN 130:7353
ED Entered STN: 09 Oct 1998
TI Effect of **Tween 20** on Freeze-Thawing- and Agitation-Induced Aggregation of Recombinant Human Factor XIII
AU Kreilgaard, Lotte; Jones, LaToya S.; Randolph, Theodore W.; Frokjaer, Sven; Flink, James M.; Manning, Mark C.; Carpenter, John F.
CS The Department of Pharmaceutics, Royal Danish School of Pharmacy, Copenhagen, Den.
SO Journal of Pharmaceutical Sciences (**1998**), 87(12), 1597-1603
CODEN: JPMSAE; ISSN: 0022-3549
PB American Chemical Society
DT Journal
LA English
CC 63-5 (Pharmaceuticals)
AB Agitation- and freeze-thawing-induced aggregation of recombinant human factor XIII (rFXIII) is due to interfacial adsorption and denaturation at the air-liquid and ice-liquid interfaces. The aggregation pathway proceeds through soluble aggregates to formation of insol. aggregates regardless of the denaturing stimuli. A nonionic surfactant, Tween 20, greatly reduces the rate of formation of insol. aggregates as a function of surfactant concentration, thereby stabilizing native rFXIII. Maximum protection occurs at concns. close to the critical micelle concentration (cmc), independent of initial protein concentration To study the mechanistic aspects of the surfactant-induced stabilization, a series of spectroscopic studies were conducted. ESR spectroscopy indicates that binding is not occurring between Tween 20 and either the native state or a folding intermediate state of rFXIII. Further, CD spectroscopy suggests that Tween 20 does not prevent the secondary structural changes induced upon guanidinium hydrochloride-induced unfolding. Taken together, these results imply that Tween 20 protects rFXIII against freeze-thawing- and agitation-induced aggregation primarily by competing with stress-induced soluble aggregates for interfaces, inhibiting subsequent transition to insol. aggregates.
ST Tween 20 aggregation recombinant human factor XIII; freeze thawing aggregation recombinant human factor XIII
IT Aggregates
Aggregation
Circular dichroism spectroscopy
Critical micelle concentration
ESR spectroscopy
Freeze drying
(Tween 20 effect on freeze-thawing-induced aggregation of recombinant human factor XIII)
IT 9013-56-3, Blood coagulation factor XIII
RL: PEP (Physical, engineering or chemical process); PRP (Properties); THU

(Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(Tween 20 effect on freeze-thawing-induced aggregation of recombinant human factor XIII)
IT 9005-64-5, Tween 20
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Tween 20 effect on freeze-thawing-induced aggregation of recombinant human factor XIII)
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L80 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:137145 HCAPLUS
DN 128:280456
ED Entered STN: 09 Mar 1998
TI **Spectroscopic probes** of the interactions of the dye Stains-all with deoxycholate and cholate
AU Goswami, Arup; Kanta Pal, Medini
CS Biophysics, Department of Biochemistry, University of Kalyani, Kalyani-741235, India
SO Colloids and Surfaces, B: Biointerfaces (**1998**), 10(3), 149-159
CODEN: CSBBEQ; ISSN: 0927-7765
PB Elsevier Science B.V.

DT Journal
LA English
CC 9-5 (Biochemical Methods)
AB The biol. surfactants sodium cholate (NaC) and sodium deoxycholate (NaDC) differ from the normal surfactants such as SDS by having hydrophilic -OH groups in their hydrophobic moieties, and they failed to induce sharp blue shifted metachromasia in the common cationic dyes such as acridine orange, methylene blue, pinacyanol etc. However, both the cholates induce extremely sharp and stable blue-shifted metachromasia in the cyanine dye Stains-all (Stal), at concentrate much below the critical micellar concns. and not disrupted by the excess of surfactants unless at above the resp. critical micellar concns. Both chiral cholates induce very strong biphasic neg. CD in Stal. At high surfactant dye both NaDC-Stal and NaC-Stal exhibit a second pos. biphasic CD spectrum, indicating the formation of second species of the complexes, not immediately discernible from the resp. absorption spectrum. Though the reported structures of micelles and crystals of NaDC are distinctly different from that of NaC, the induced metachromasia and CD in Stal by the two surfactants are remarkably similar. It is reasonably thought that Stal cations bound at NaC and NaDC are arranged with systematic twists in one sense, responsible for metachromasia and dichroism of the dye aggregates, the formation of NaDC-Stal and NaC-Stal are probably followed by some self organization of the complexes formed in the premicellar range of concns., excess surfactants added to these complexes form just part of the solvent. Only above cmc the micelles start disruption of the dye aggregates. Our results fit well with the helical model of NaDC and the Small's model of NaDC micellar aggregate with the hydrophobic surfaces oriented inside.
ST spectroscopy probe interaction dye Stains all; deoxycholate cholate
IT **Circular dichroism**
Critical micelle concentration
UV and visible spectroscopy
(spectroscopic probes of interactions of dye Stains-all with deoxycholate and cholate)
IT 7423-31-6, Stains-all
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(spectroscopic probes of interactions of dye Stains-all with deoxycholate and cholate)
IT 302-95-4, Sodium deoxycholate 361-09-1, Sodium cholate
RL: RCT (Reactant); RACT (Reactant or reagent)
(spectroscopic probes of interactions of dye Stains-all with deoxycholate and cholate)
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L80 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:537650 HCAPLUS
DN 127:201665
ED Entered STN: 23 Aug 1997
TI Effects of temperature and concentration on **bovine lens** α-crystallin secondary structure: a circular dichroism spectroscopic study
AU Farnsworth, Patricia N.; Groth-Vasselli, B.; Greenfield, Norma J.; Singh, Kamalendra
CS Department of Pharmacology and Physiology, UMD-New Jersey Medical School, Newark, NJ, 07103, USA
SO International Journal of Biological Macromolecules (**1997**), 20(4), 283-291
CODEN: IJBMDR; ISSN: 0141-8130
PB Elsevier
DT Journal
LA English
CC 6-3 (General Biochemistry)
AB Elucidation of the structure of α-crystallin, the major protein in all vertebrate lenses, is important for understanding its role in maintaining transparency and its function in other tissues under both normal and pathol. conditions. Progress toward a unified consensus concerning the tertiary and quaternary structures of α-crystallin depends, in part, on an accurate estimation of its secondary structure. For the first time, three algorithms, SELCON, K2D and CONTIN were used to analyze far ultra-violet CD (UV-CD) spectra of bovine lens α-crystallin to estimate the secondary structure and to determine the effects of temperature and concentration Under all exptl. conditions tested, the analyses show that α-crystallin contains 14% α-helix, 35% β-sheet and the remainder, random coil and turns. The results suggest that